

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057120.D
 Acq On : 21 Dec 2023 03:45
 Operator : MD/SY
 Sample : 05892-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B09

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.534	61	76	96	rBV	264082	967831	100.00%	12.563%
2	2.001	215	221	236	rVB2	164656	281937	29.13%	3.660%
3	2.078	240	245	260	rVB2	102997	183412	18.95%	2.381%
4	2.152	263	268	279	rVB	68018	100926	10.43%	1.310%
5	2.666	414	428	444	rBV3	268713	554545	57.30%	7.198%
6	2.888	491	497	515	rVB	9068	15193	1.57%	0.197%
7	3.984	827	838	853	rVB2	19521	45335	4.68%	0.588%
8	4.753	1065	1077	1087	rBV2	18773	43298	4.47%	0.562%
9	5.136	1183	1196	1214	rVB	133171	290006	29.96%	3.764%
10	5.795	1386	1401	1424	rVB2	242743	600427	62.04%	7.794%
11	6.373	1566	1581	1598	rBV	225911	432824	44.72%	5.618%
12	6.653	1658	1668	1682	rVB5	11515	20597	2.13%	0.267%
13	6.795	1696	1712	1728	rBV2	143099	284305	29.38%	3.690%
14	7.634	1960	1973	1990	rBV2	63059	116412	12.03%	1.511%
15	7.955	2061	2073	2088	rBV	262724	478774	49.47%	6.215%
16	8.229	2149	2158	2170	rBV3	36140	63434	6.55%	0.823%
17	8.383	2198	2206	2216	rBV3	19909	34406	3.55%	0.447%
18	8.508	2236	2245	2255	rVB5	12895	21881	2.26%	0.284%
19	8.685	2286	2300	2326	rBV	184280	437001	45.15%	5.672%
20	9.444	2523	2536	2571	rVB	299651	575933	59.51%	7.476%
21	10.766	2932	2947	2961	rBV	85542	145966	15.08%	1.895%
22	10.894	2977	2987	3000	rVB2	12069	22214	2.30%	0.288%
23	11.695	3226	3236	3245	rBV9	9302	17491	1.81%	0.227%
24	11.746	3245	3252	3261	rVV8	9050	15791	1.63%	0.205%
25	11.817	3261	3274	3294	rVV	296557	532582	55.03%	6.913%
26	11.981	3320	3325	3341	rVB	4772	10724	1.11%	0.139%
27	12.193	3374	3391	3411	rVB	254241	457001	47.22%	5.932%
28	12.888	3595	3607	3616	rVB8	13801	21337	2.20%	0.277%
29	12.974	3623	3634	3645	rBV8	11845	20234	2.09%	0.263%
30	15.093	4284	4293	4305	rBV2	16846	26558	2.74%	0.345%
31	15.396	4376	4387	4401	rVB8	10805	18220	1.88%	0.236%
32	15.685	4463	4477	4489	rBV5	38818	66264	6.85%	0.860%
33	15.936	4544	4555	4569	rBV	233472	361545	37.36%	4.693%
34	16.125	4604	4614	4619	rBV10	7135	11285	1.17%	0.146%
35	16.759	4801	4811	4821	rBV2	125107	191322	19.77%	2.483%
36	16.878	4834	4848	4866	rBV	117309	195733	20.22%	2.541%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Title : TRACE VOA SFAM1.0

37	17.460	5022	5029	5043	rBV	17988	41328	4.27%	0.536%
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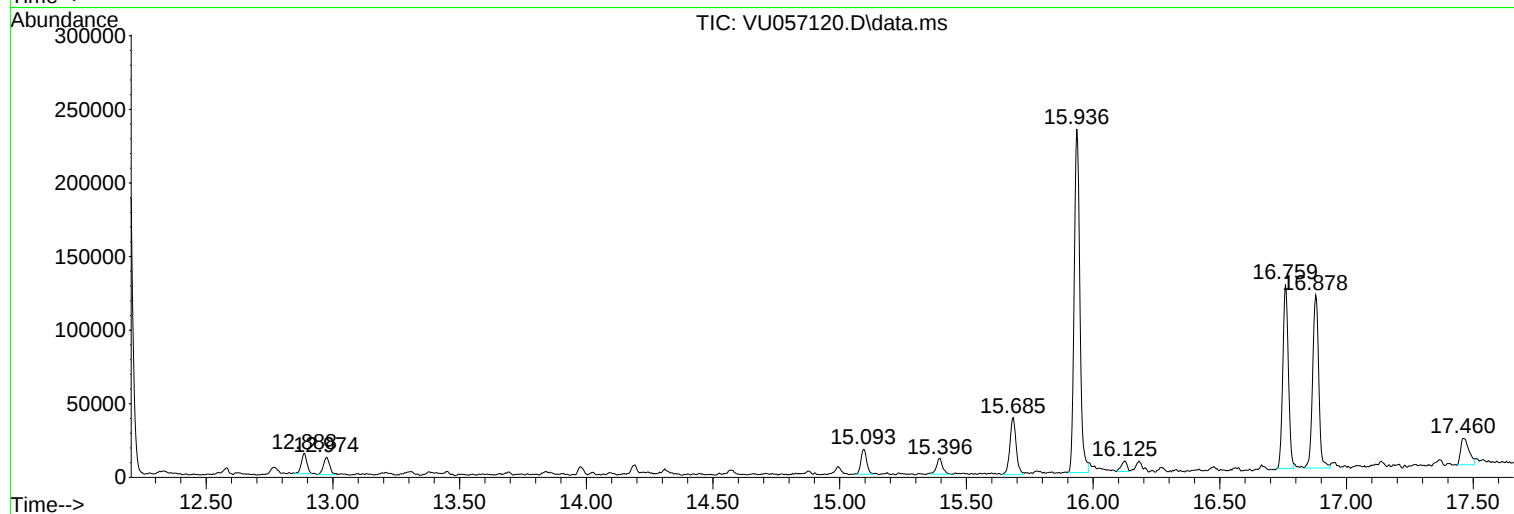
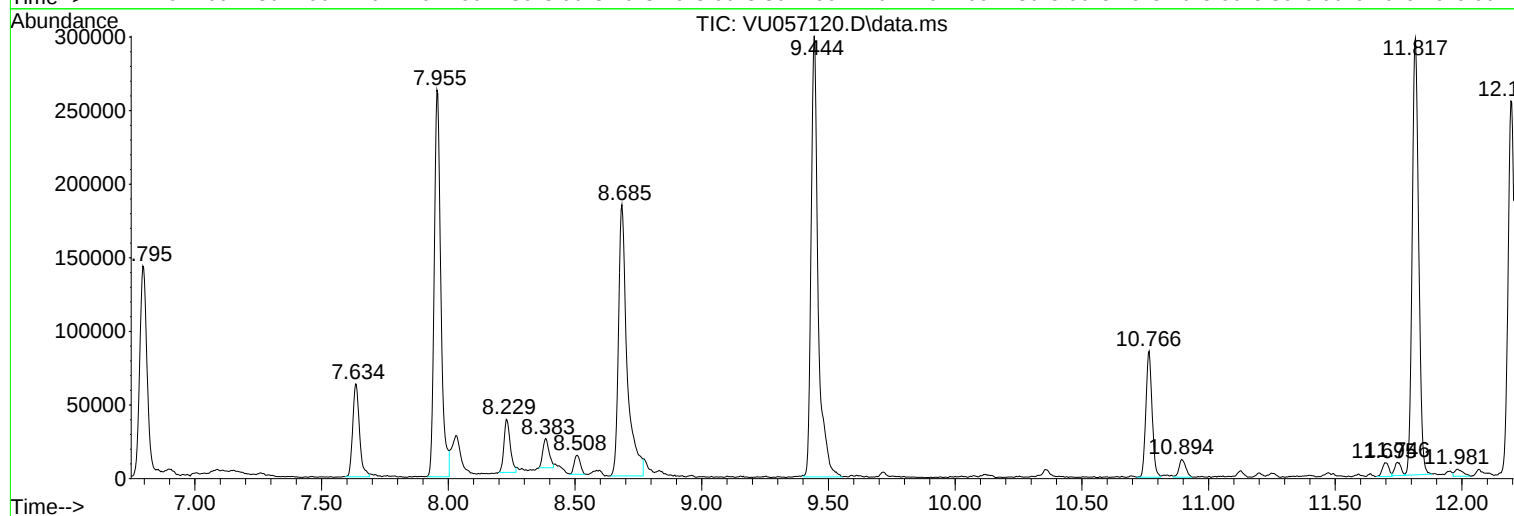
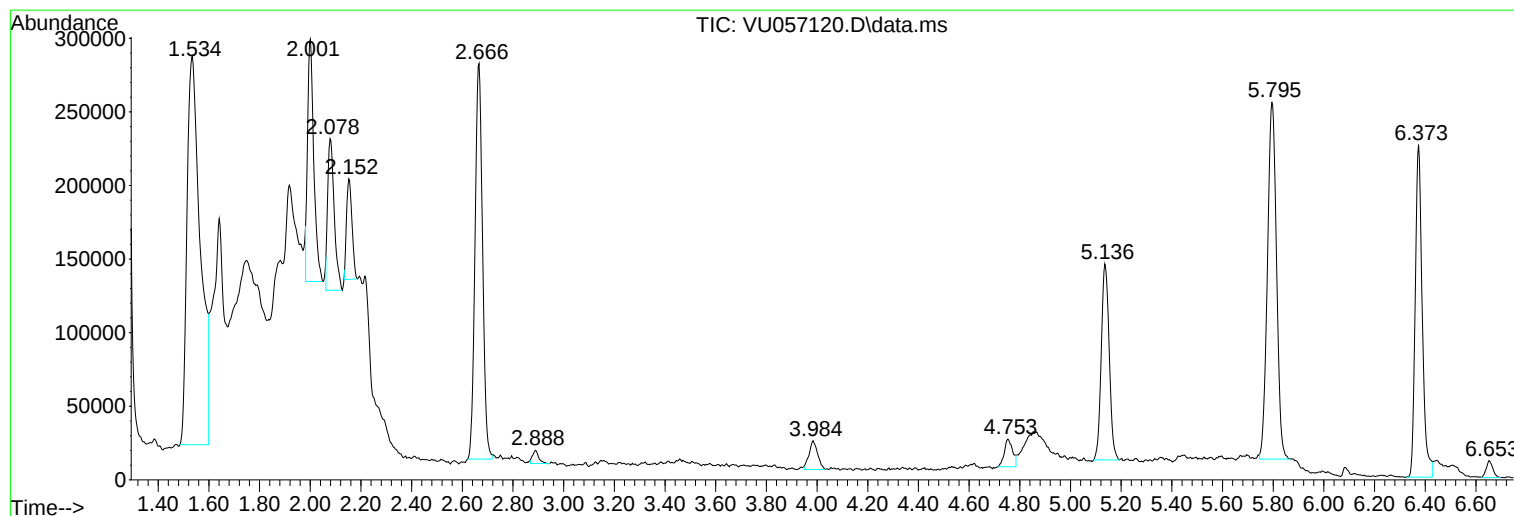
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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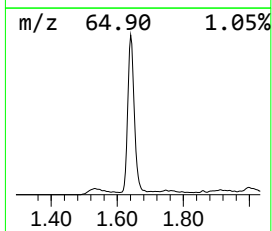
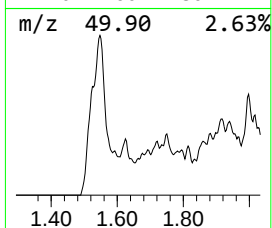
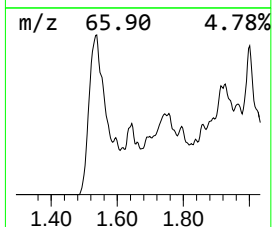
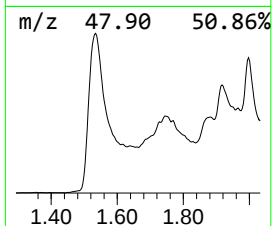
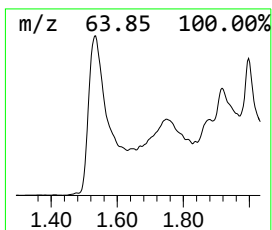
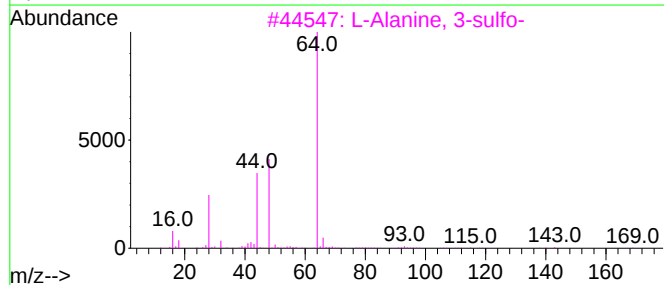
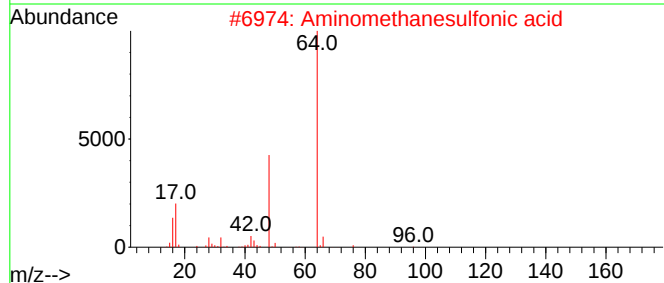
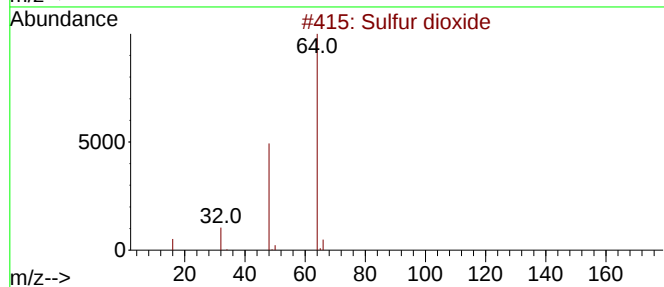
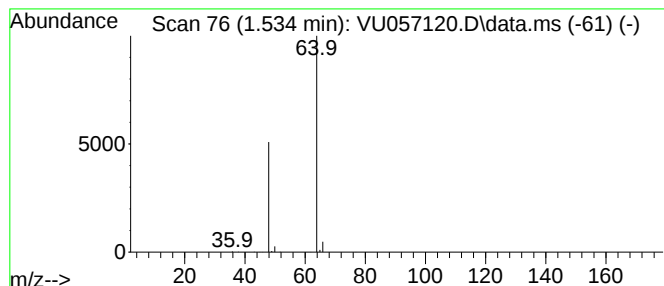
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.534	11.18 ug/L	967831	1,4-Difluorobenzene	6.373

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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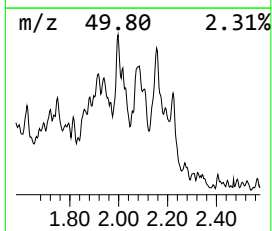
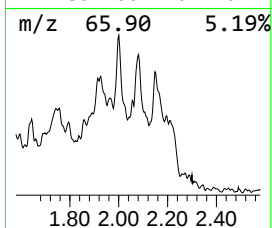
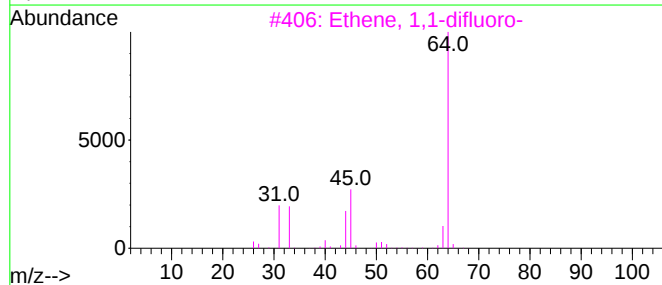
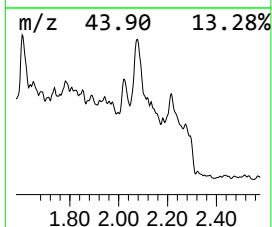
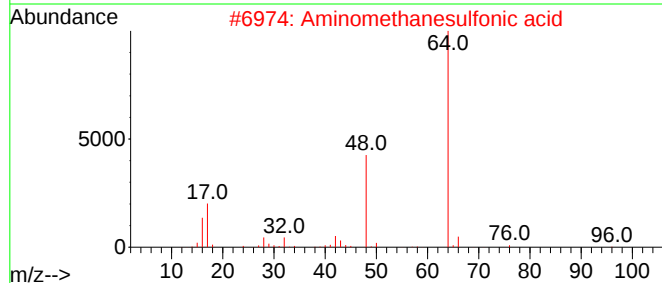
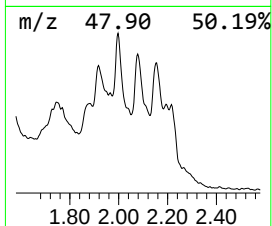
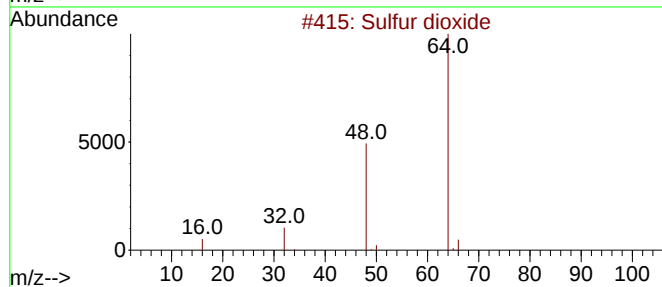
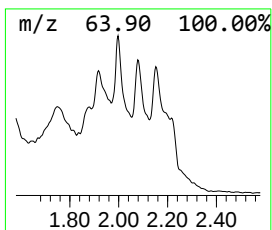
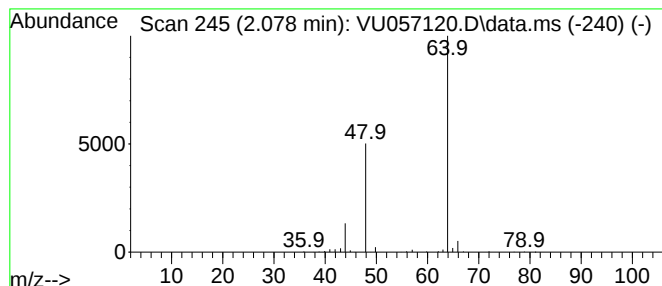
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.078	2.12 ug/L	183412	1,4-Difluorobenzene	6.373

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	56
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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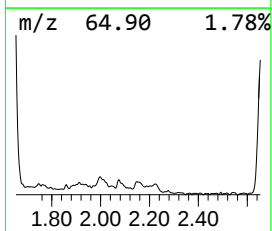
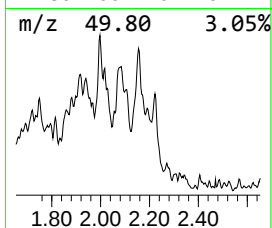
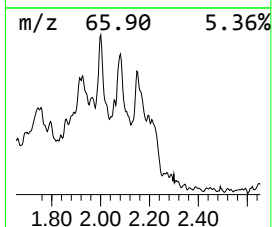
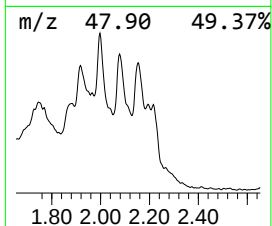
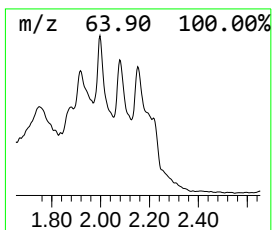
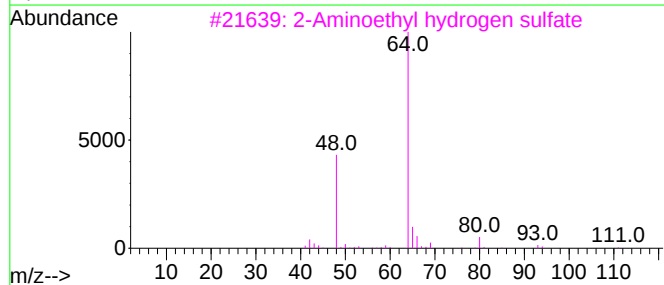
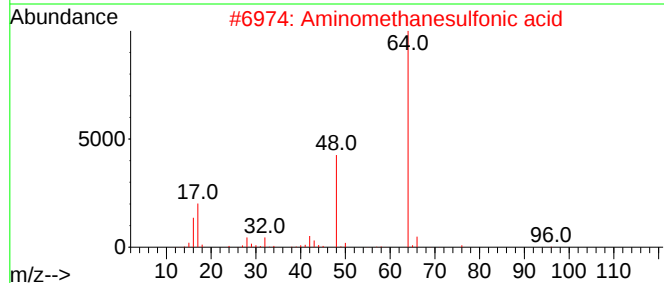
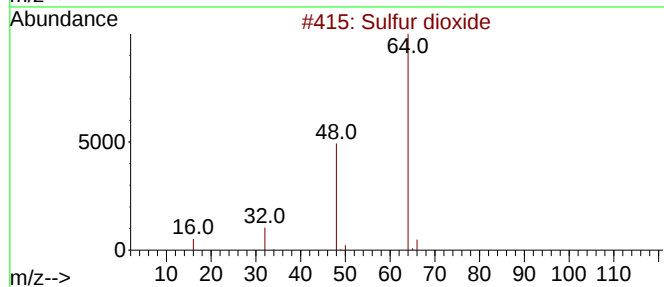
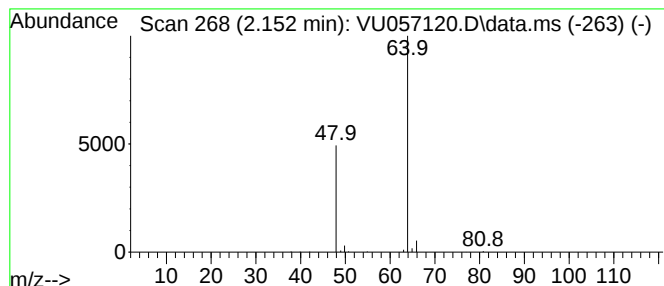
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Aminoethyl hydrogen sulfate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	1.17 ug/L	100926	1,4-Difluorobenzene	6.373

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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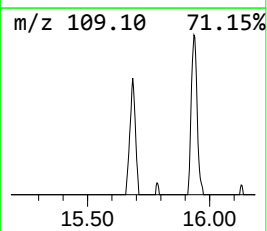
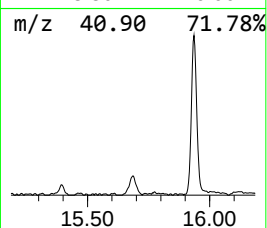
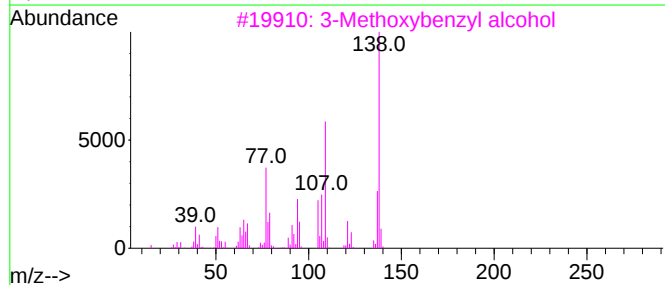
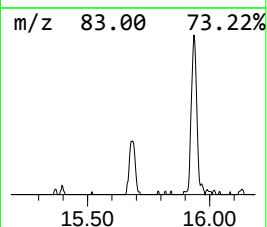
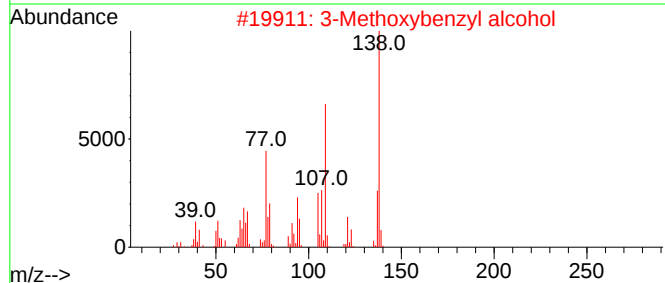
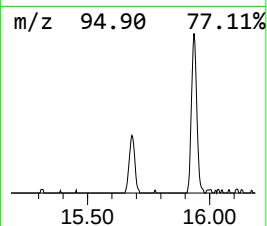
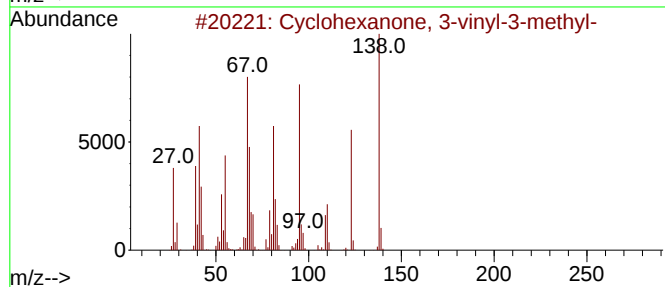
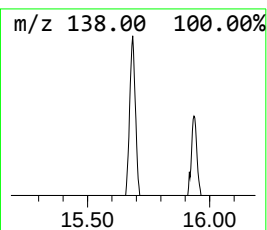
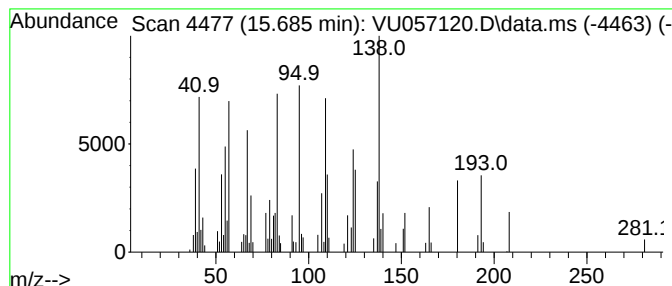
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.685	0.62 ug/L	66264	1,4-Dichlorobenzene-d4	11.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3-vinyl-3-methyl-	138	C9H14O	068269-56-7	38
2			3-Methoxybenzyl alcohol	138	C8H10O2	006971-51-3	35
3			3-Methoxybenzyl alcohol	138	C8H10O2	006971-51-3	35
4			2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	25
5			Cyclopentanecarboxaldehyde, 2-me...	124	C8H12O	1000154-24-0	25



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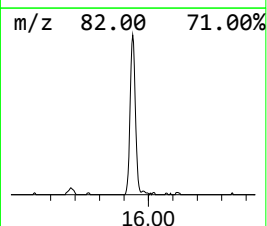
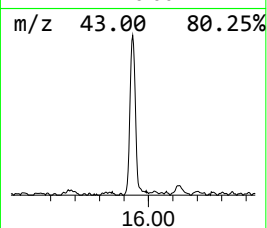
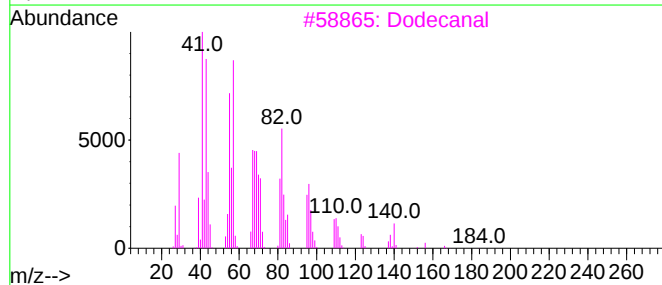
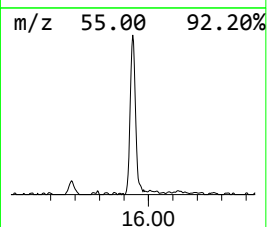
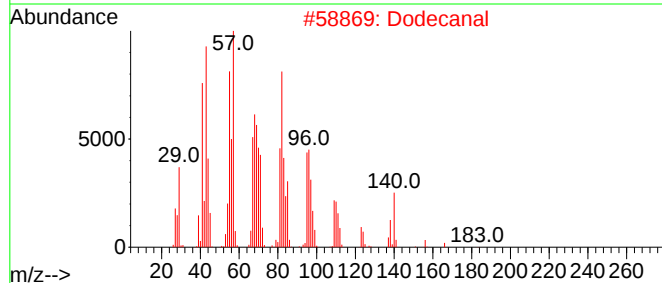
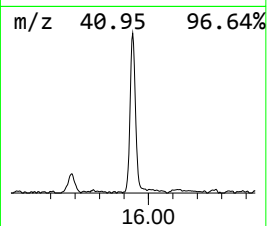
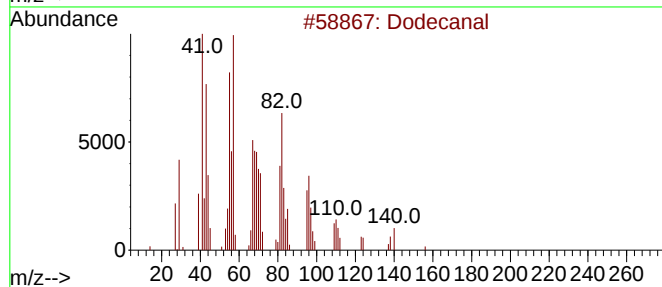
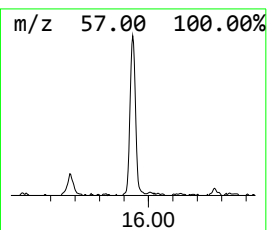
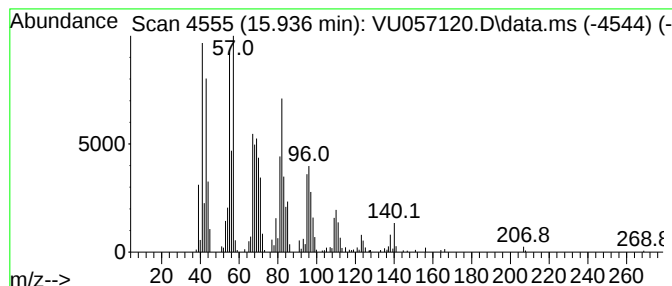
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.936	3.39 ug/L	361545	1,4-Dichlorobenzene-d4	11.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanal			184	C12H24O	000112-54-9	93
2	Dodecanal			184	C12H24O	000112-54-9	91
3	Dodecanal			184	C12H24O	000112-54-9	91
4	Tetradecanal			212	C14H28O	000124-25-4	90
5	Tridecanal			198	C13H26O	010486-19-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
Data File : VU057120.D
Acq On : 21 Dec 2023 03:45
Operator : MD/SY
Sample : 05892-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7B09

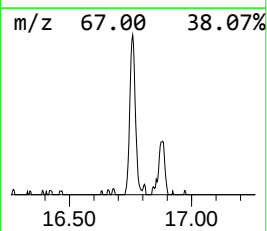
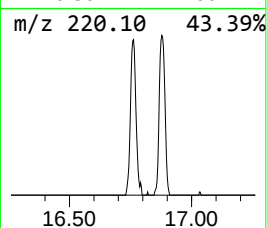
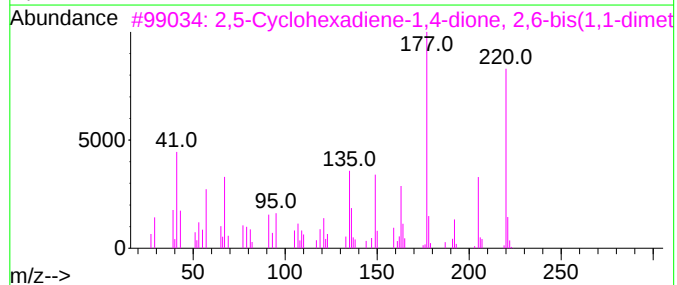
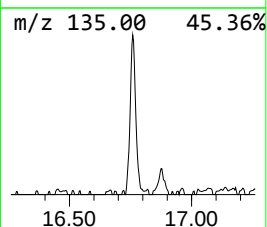
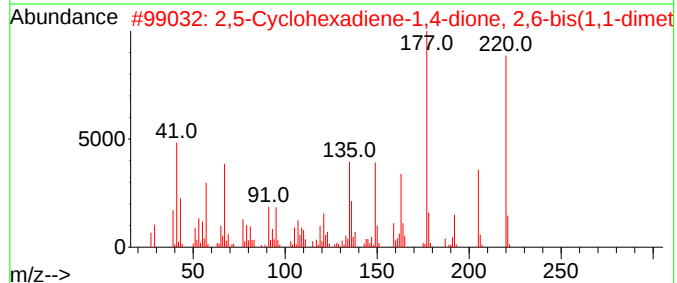
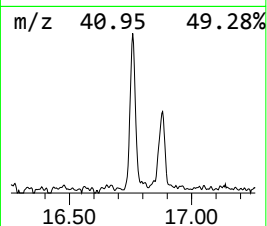
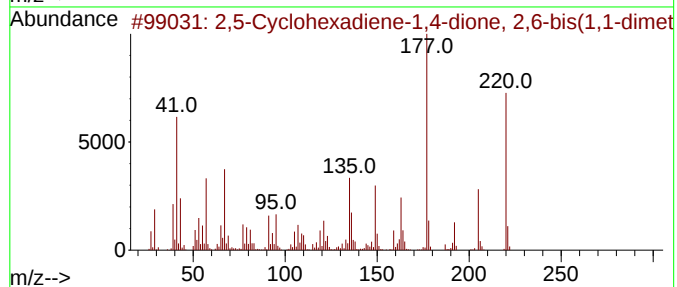
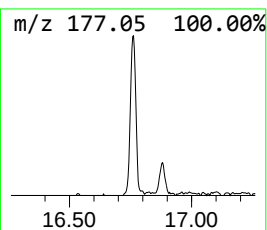
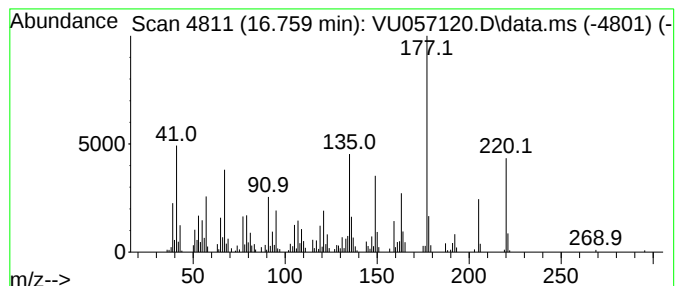
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.759	1.80 ug/L	191322	1,4-Dichlorobenzene-d4	11.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
Data File : VU057120.D
Acq On : 21 Dec 2023 03:45
Operator : MD/SY
Sample : 05892-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7B09

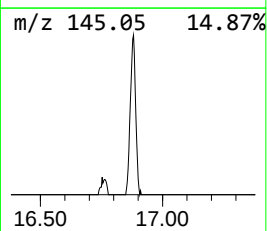
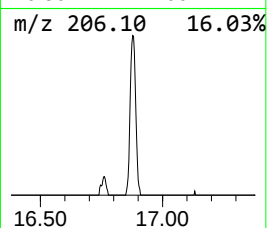
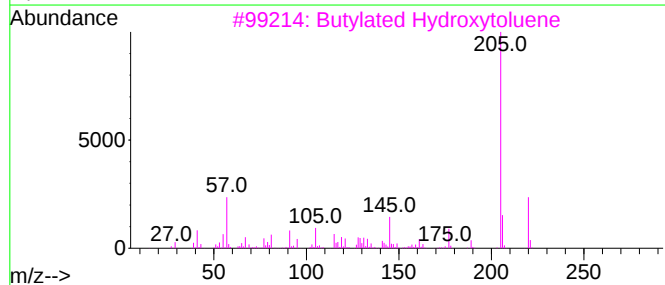
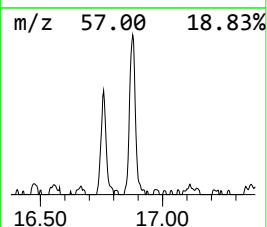
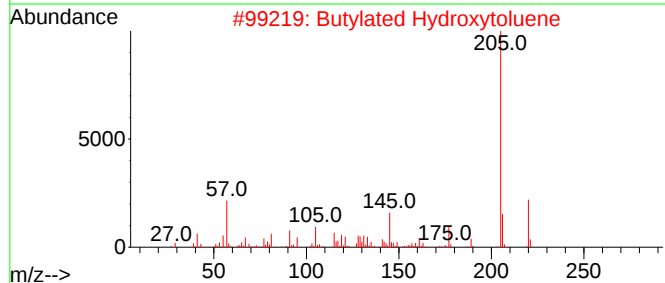
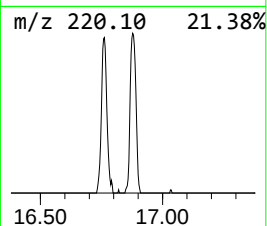
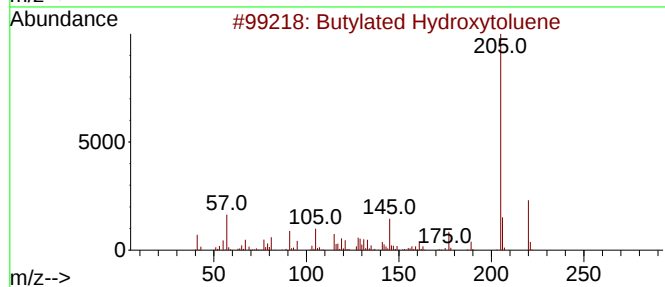
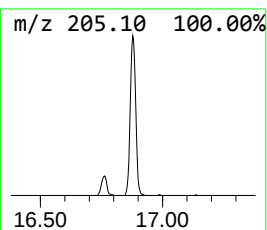
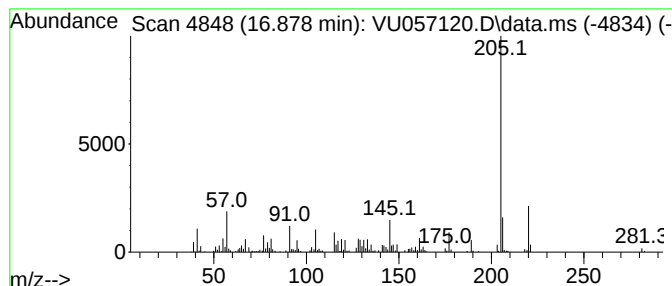
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Butylated Hydroxytoluene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.878	1.84 ug/L	195733	1,4-Dichlorobenzene-d4	11.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
Data File : VU057120.D
Acq On : 21 Dec 2023 03:45
Operator : MD/SY
Sample : 05892-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7B09

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.534	11.2	ug/L	967831	1	6.373	432824	5.0
Aminomethanesul...	2.078	2.1	ug/L	183412	1	6.373	432824	5.0
2-Aminoethyl hy...	2.152	1.2	ug/L	100926	1	6.373	432824	5.0
unknown-01	15.685	0.6	ug/L	66264	3	11.817	532582	5.0
Dodecanal	15.936	3.4	ug/L	361545	3	11.817	532582	5.0
2,5-Cyclohexadi...	16.759	1.8	ug/L	191322	3	11.817	532582	5.0
Butylated Hydro...	16.878	1.8	ug/L	195733	3	11.817	532582	5.0